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Final Report

"Characterization of Boron Atom Aggregation" (SPC 00-4073)

The project was primarily aimed at obtaining electronic spectra of boron aggregates. A unique facility is available for this; an apparatus developed in Basel during the last decade which combines mass-selection with matrix isolation spectroscopy. Figure 1 shows the concept of this complex instrument.

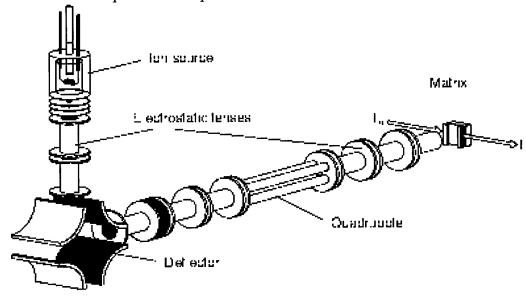


Figure1.

An objective set for the six month period (1.October 2000- 31. March 2001) of the project was achieved, in that the electronic spectra of B₃ and B₃ in a neon matrix could be observed for the first time. In the initial submission, finances for a year's project including support for a PhD student were requested. However, as the amount available was \$15'000.- the project was rescaled for about a 6 month period: the salary for a PhD student in Switzerland is around \$20'000 per year. Muriel Wyss and Evgueni Riaplov were the students who worked on this project during this period. Collaboration, consultation and exchange of information was maintained with Dr.C.W.Larson of the Air Force Research Laboratory, Edwards, AFB.

The B_3 molecule plays a key role in the characterization of boron "High Energy Density Matter". It has been theorized that B_3 may be an "island of stability" in boron High Energy Density Matter because it may resist attack by B and B_2 to form higher clusters. Thus the observation of the electronic spectrum is an important step for the further experimental investigations. To obtain the spectra, B_3^- anions produced by cesium sputtering on a boron carbide rod were mass-selected and codeposited with neon on a 5 K surface to grow a matrix. In this the B_3^- anions are trapped as isolated entities. The absorption of B_3^- is observed with origin band at 448 nm (figure 2) and is the $A^- \Pi_u$ - $^1\Sigma_g^+$ electronic transition.

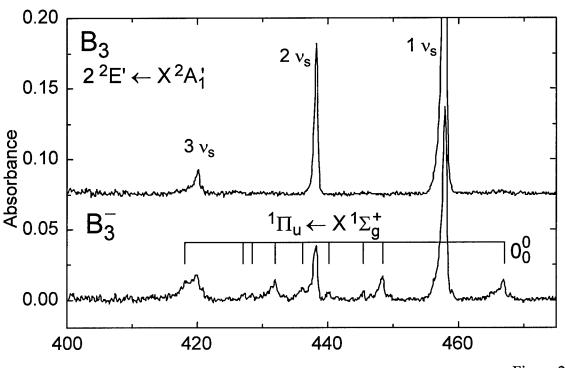


Figure 2.

The anion is then converted through photolysis to B_3 in the matrix and shows two electronic transitions, one with origin band at 736 nm ($1^2E^{'}-X^2A_1^{'}$ figure 2) and other at 458 nm ($2^2E^{'}-X^2A_1^{'}$ figure 3).

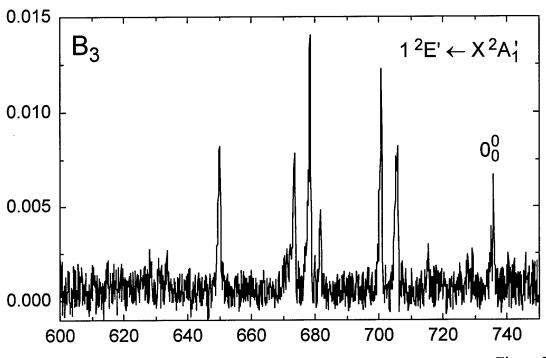


Figure 3.

An article reporting these new spectra is being prepared. However, the interpretation of the vibrational structure of the spectra requires theoretical support: the excited electronic states are degenerate and subject to a Jahn-Teller distortion. The theory for this is being developed by the group of Prof.P.Rosmus, Universite de Marne la Vallee, France, with whom we have a collaboration.

Experiments were also attempted to observe the spectra of B_4 , using mass-selected B_4 , so far without success. This is associated with inadequate ion currents, 0.5 nA for B_4 has been the best attained, and will require in the future source development, including perhaps the use of boron complexes as precursors.

The first experiments to follow boron atom aggregation were also attempted. In this, mass-selected B⁻ atoms were codeposited with neon and the matrix was warmed up from 4 to 8 K. This increases the mobility of the boron atoms causing the formation of boron molecules. The ready formation of the molecule OBO was observed. It is produced because of trace amounts of oxygen in the neon matrix.

(1) "The Contractor, Institute for Physical Chemistry, hereby declares that, to the best of its knowledge and belief, the technical data delivered herewith under contract No. F61775-00-WE073 is complete, accurate and complies with all the requirements of the contract."

DATE 14. May, 2001

Name and Title of Authorized official: John P.Maier, Professor, Director of Institute of Physical Chemistry "

(2) **(B)** "I certify that there were no subject inventions to declare as defined in FAR 52.227-13, during the performance of this contract."

DATE 14. May, 2001

Name and Title of Authorized official: John P.Maier, Professor, Director of Institute of Physical Chemistry "

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